The conductance of nanotubes deformed by the AFM tip

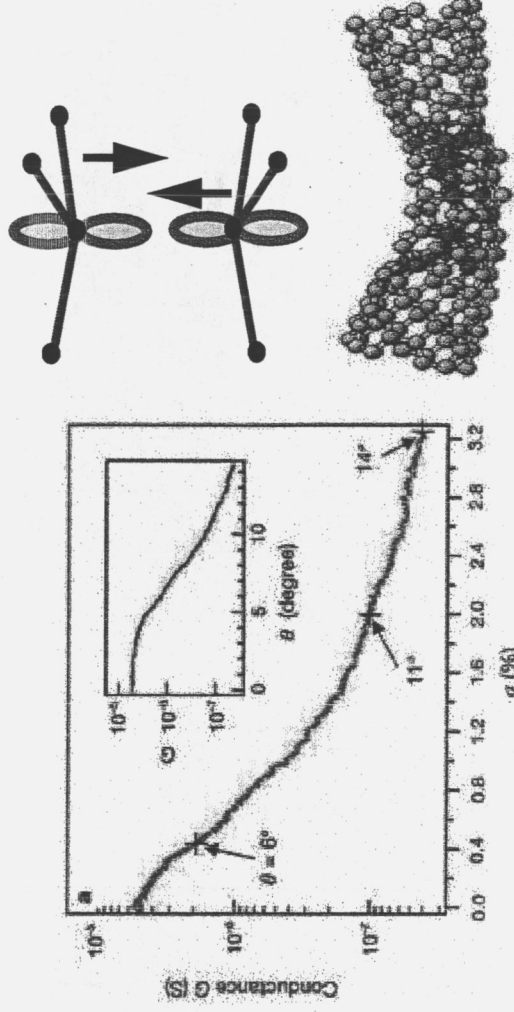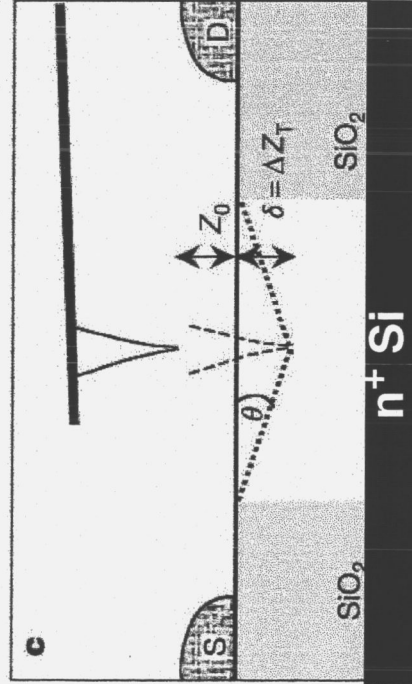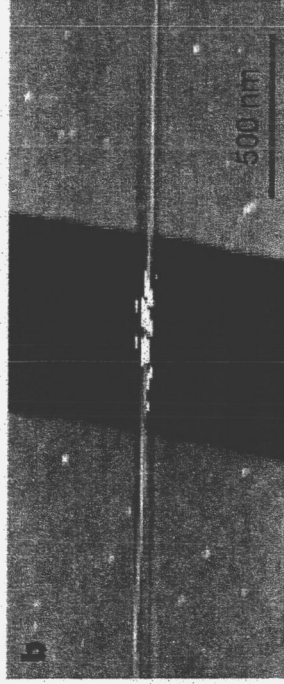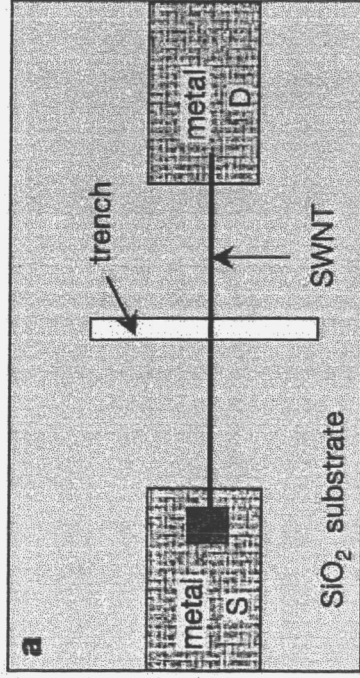Alexei Svizhenko[1], Amitesh Maiti[2], M. P. Anantram[1],

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NASA Ames Research Center

Motivation

T. W. Tombler et al, Nature 405, 769 (2000).

SWNT deformed by AFM tip shows a drop in conductance by 2 orders of magnitude, which was explained as the effect of sp3-bonding

Drop in conductance can also be due to the tensile stretching *Maiti et al., PRL 88, 126805 (2002)*

Can stretching alone fully explain the experiment?

Can sp3-bonding alone decrease the conductance in nanotubes ?

Outline:

- ## Simulations of the experiment

  - ### Technique

- ## Effect of diameter, length and temperature

- ## Study of sp3 coordination- "The Table experiment"

  - ### Effect of elastic deformation

  - ### Forming of sp3 bonds

  - ### Breaking the bonds

  - ### Effect of the AFM tip

- ## Conclusion

Our simulations:

- **Structure:**
  - Molecular Dynamics+DFT (Accelrys' DMol^3):

- **Transport**
  - Non-orthogonal sp^3 tight-binding Hamiltonian (1. *D.A.Papaconstantopoulos et al. or 2. Charlier et al.*). Effect of deformation: $H_{12}(r)$, $S_{12}(r) \sim (r_o/r)^2$
  - Two terminal device - Hamiltonian is a block-tridiagonal matrix
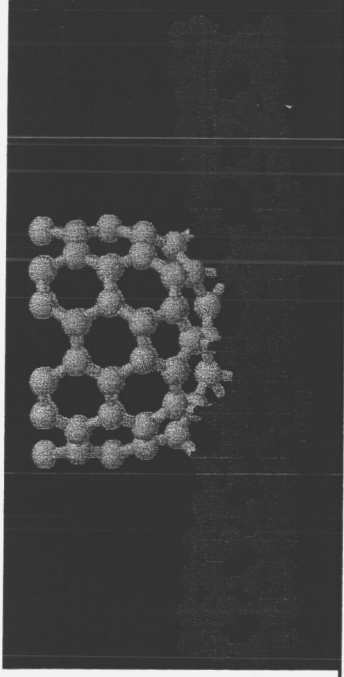 - Three terminal device - Hamiltonian is a full matrix.

$$(E \cdot S_{ij} - H_{ij} - \Sigma^R_{L,ij} - \Sigma^R_{R,ij} - \Sigma^R_{T,ij})G^{R,jk}_j = \delta^k_i$$

$$T_{c1c2}(E) = G^{R,ij} G_{c1,jk} G^{A,kl} G_{c2,li}, \quad c1,c2 = L,R,T$$
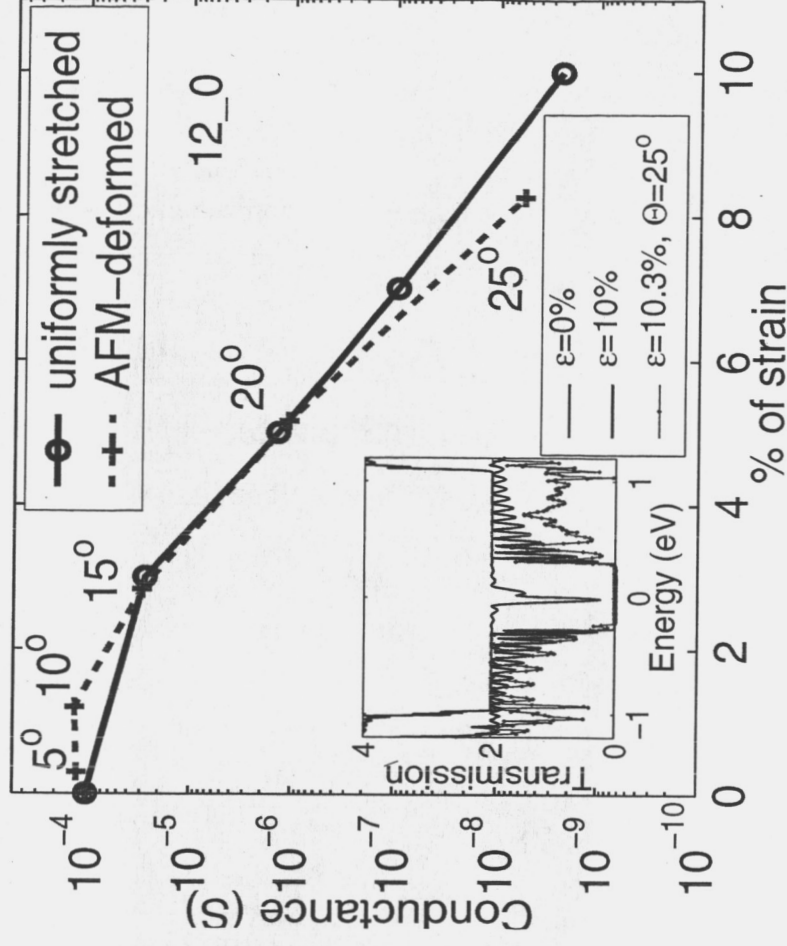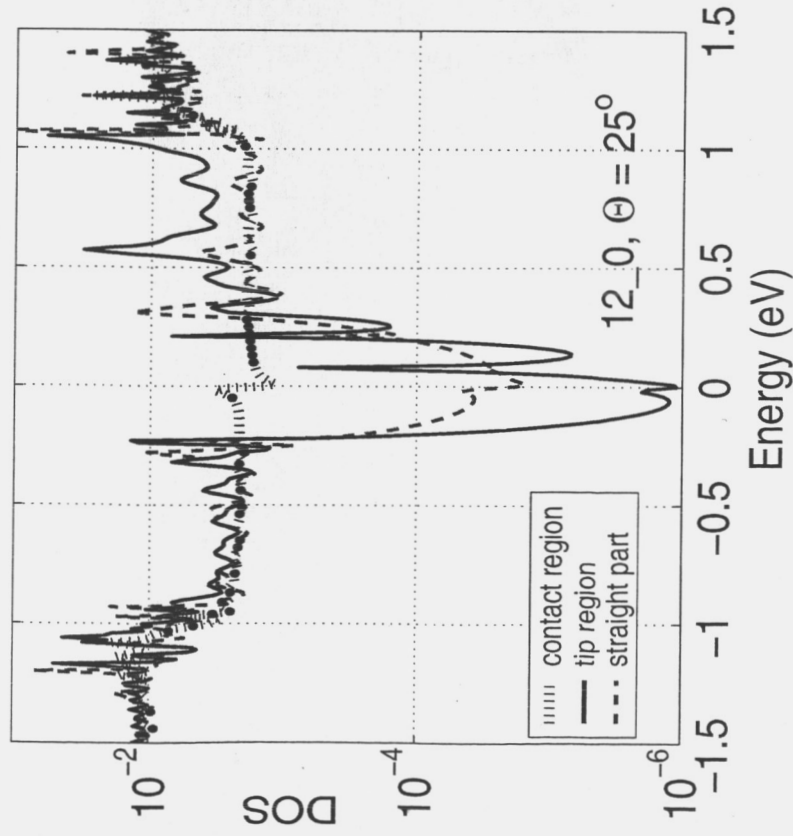
Σ^R_T:

Σ^R_L

...

Σ^R_R

...

$$G = \frac{2e^2}{h} \int_{-\infty}^{\infty} T(E)\left(-\frac{\partial f_o}{\partial E}\right)dE$$

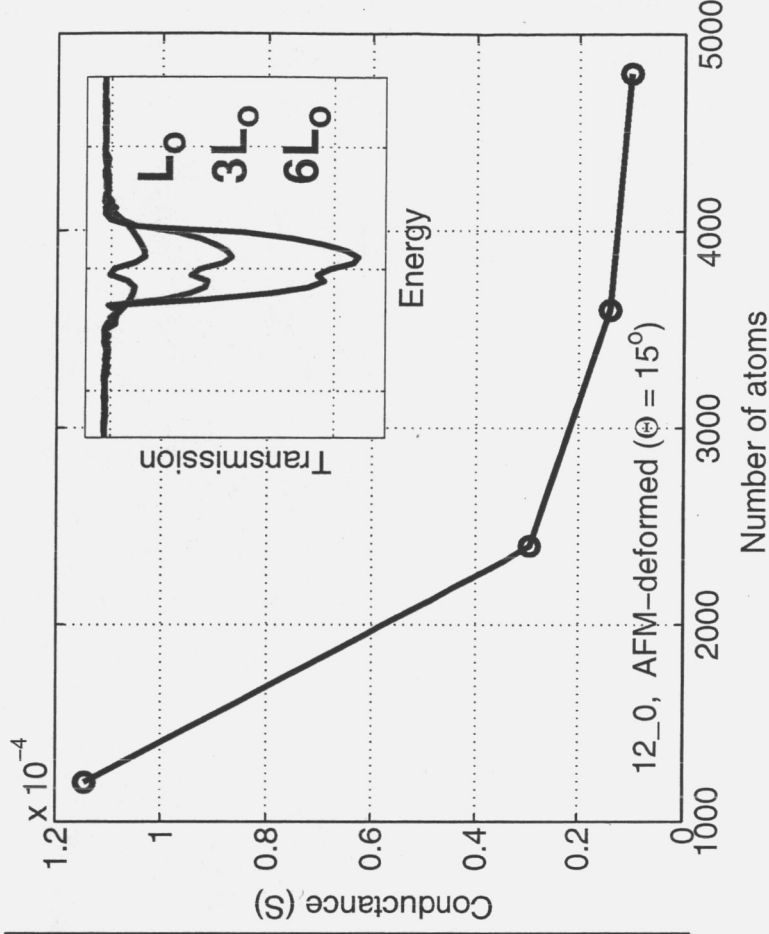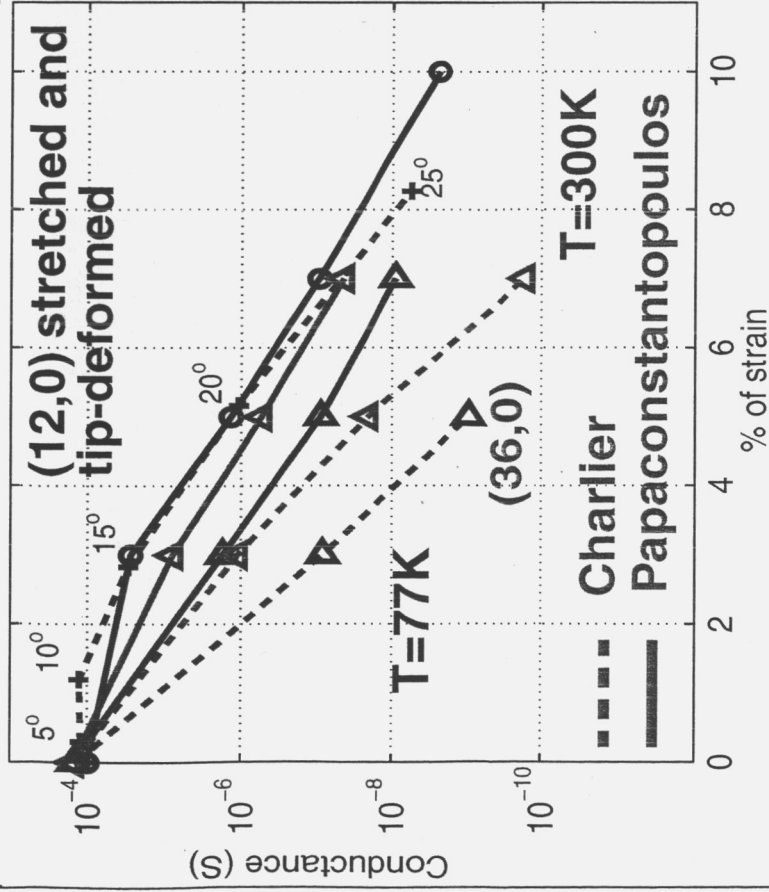# Bandgap in zigzag nanotube uner AFM-tip deformation

- **Conductance drop occurs in tip region and straight parts due to stretching**

- **Chirality dependent: maximum for zigzag, zero for armchair**

Maiti et al., PRL 88, 126805 (2002)

Effect of diameter, length, temperature and TB parametrization

- **Can stretching explain 2 orders drop in conductance @ $\Theta=15°$ or 3%?**

- In (12,0) tube conductance drops by a factor of 3 ($\Theta=15°$ or 3% strain)

- Diameter: In (36,0) tube (3nm in diameter) conductance drops by a factor of 19.8

- Length: in a longer (36,0) tube conductance drops by a factor of 59

- TB parametrization: more sensitive scheme by Charlier results in a drop by 87 (dashed red line)

- Temperature: at T=293K , (36,0) with Charlier parameters the drop wil be 96

- For longer and thicker tubes, the drop may be higher than 10^2 , which sugests chiral tube may have been involved in the experiment.

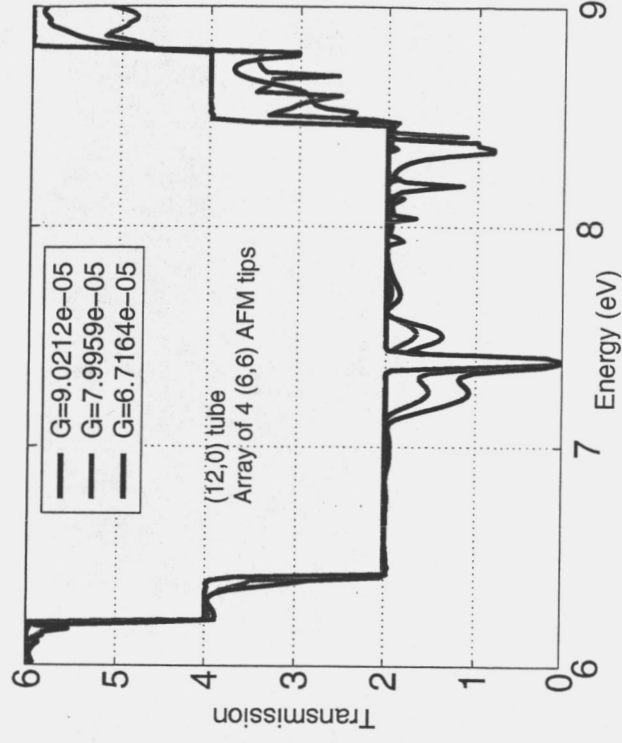NASA Ames Research Center
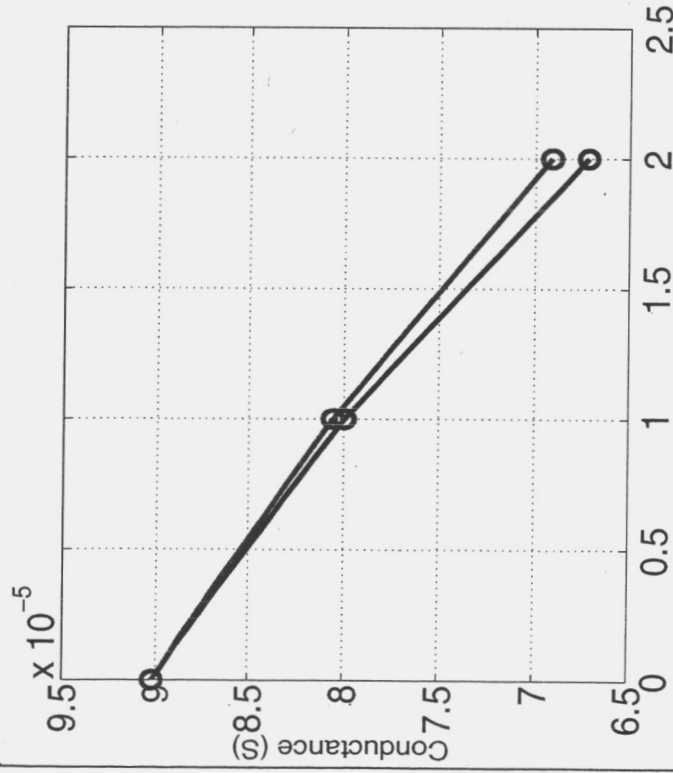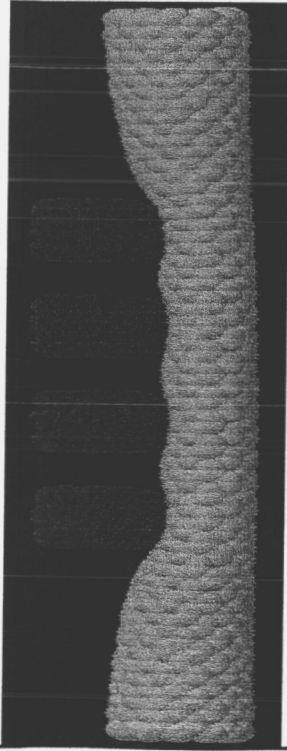
The "Table experiment"
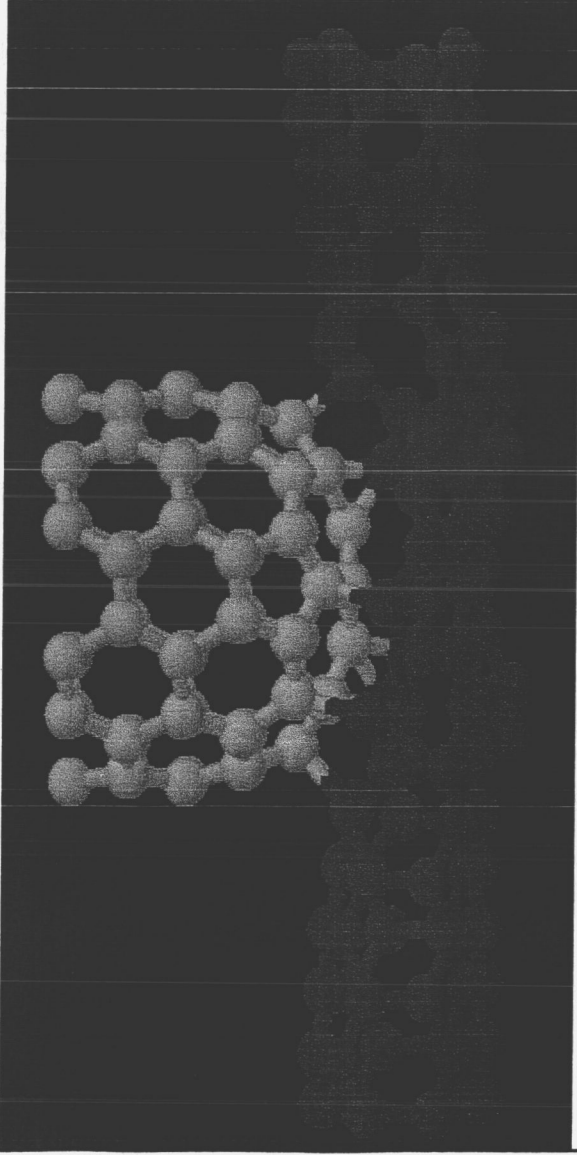
A nanotube lying on the table is deformed by an AFM tip

Typical system : (3,3) tube and (6,6) tip

- What is the effect of deformation on conductance?

  - Elastic deformation
  - Formation of sp3 bonds
  - Breaking the bonds
  - What is the effect of the AFM tip?

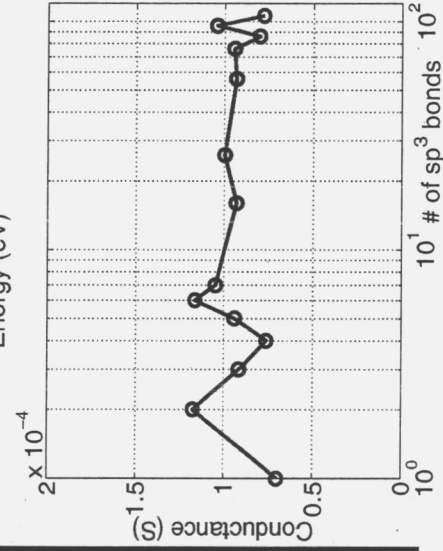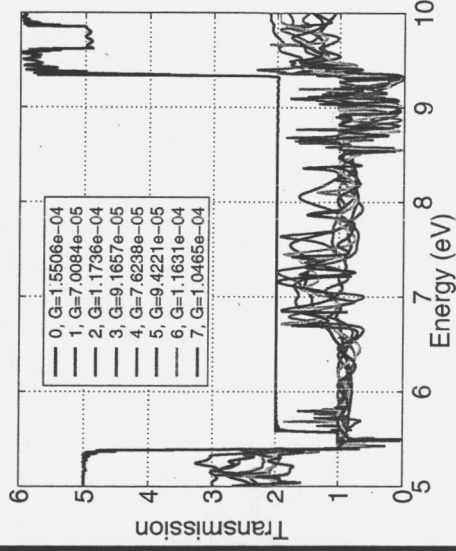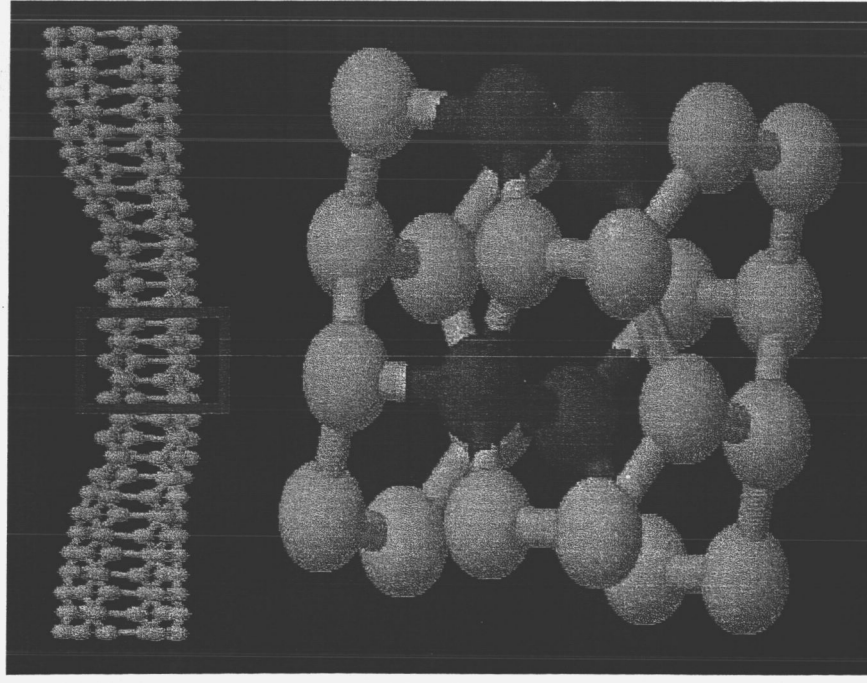# Elestic deformation by the array of AFM tips: No sp3 bonds

- Conductance drops by a factor of 1.5

Formation of the sp3 bonds

- (3,3) tube

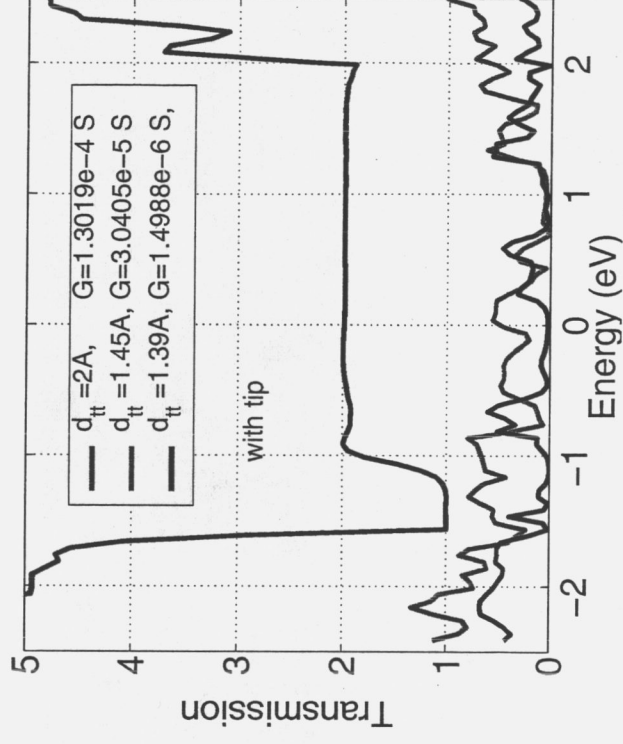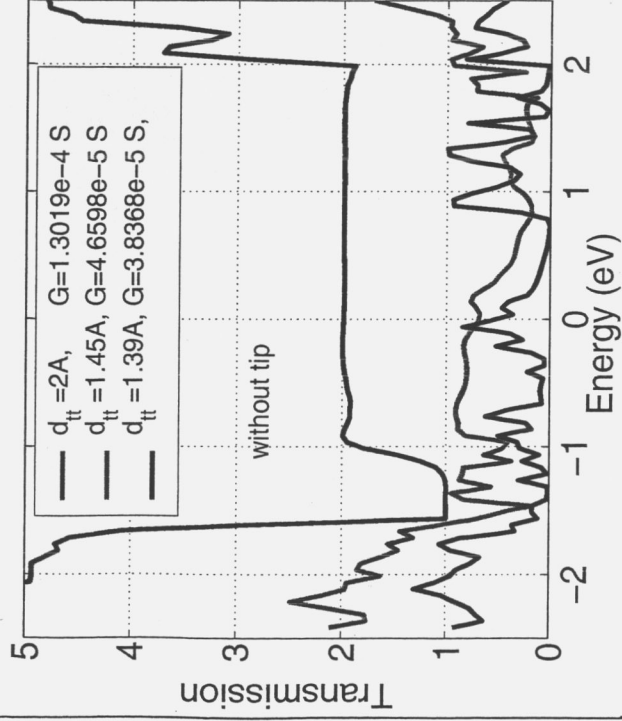- An sp3 bond between the top and bottom walls of the nanotube was formed for each unit cell, by fixing two atoms

- How does conductance depends on the number of sp3 bonds?

- Conductance does not change for tubes with up to 100 sp3 bonds

- Left and right walls remained sp2 coordinated

- Left and right walls form a conducting path for electrons , which keeps the conductance high

Broken bonds and Effect of the AFM tip

AFM tip is a (6,6) caped nanotube

Legend (without tip):
- $d_{tt} = 2A$, G=1.3019e-4 S
- $d_{tt} = 1.45A$, G=4.6598e-5 S
- $d_{tt} = 1.39A$, G=3.8368e-5 S,

Legend (with tip):
- $d_{tt} = 2A$, G=1.3019e-4 S
- $d_{tt} = 1.45A$, G=3.0405e-5 S
- $d_{tt} = 1.39A$, G=1.4988e-6 S,

- Conductance decreases only when bonds are broken

- Atoms on the tip form sp3 bonds with atoms on the tube . This decreases conductance

Conclusion:

- The conductance drop under AFM-tip deformation can be explained by stretching of the tube length. NT sensors can be built utilizing uniform stretching.

- single sp3 bond per crossection cannot block electrons, because other conducting path may exist

- AFM tip which forms sp3 bonds with the tube will decrease conductance

- In the "table experiment" conductance drop of 2 orders of magnitude happened only after some bonds are broken